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# Electronic Tuning of Intersubband Transition of Inverted Core-Shell Cylindrical Quantum Wire for Novel Lasing Performance

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## Abstract

A novel quantum wire laser structure is presented by designing inverted core-shell cylindrical quantum wire using  $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$  type-I heterostructure. The energy eigenvalues with corresponding density of states are numerically computed using finite difference technique. Intersubband transition energies are computed considering the lowest three energy states only where material composition of core material is changed to observe the effect on it. Dimensional effect is also studied for suitability of application in case of optical tuning. This analysis is carried out by taking into consideration the conduction band discontinuity and effective mass mismatch at boundaries following BenDaniel duke boundary condition. Results reflect that accuracy of control can be achieved on lasing performance by combining the dimensional variation effect with material parameter adjustment.

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**Keywords:** Finite difference technique; Energy eigenvalue; Inverted core-shell cylindrical wire; Intersubband transition energies; Density of states

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## 1. Introduction

Present day of theoretical research on low-dimensional semiconductor heterostructure is able supported by the modern microelectronics technology for fabrication [1-2], and therefore, a new era of exploring quantum electronics devices is stimulated with impetus to both theoretical and experimental works having wider perspectives. Conventional nano-heterosystems are now replaced by ultra-thin quantum structures with 2-D/3-D confinement having multiple layers which possess unique transport features along with novel electronic and photonic properties [3-5]. This becomes possible by restricting the electron motion along dimension which is made comparable to de-Bröglie's wavelength, and resulting nanowire's already made a significant contribution in the field of future VLSI devices reported by

eminent workers in recent past [4, 6-7]. Considerable attention has already been drawn by cylindrical structure for theoretical [8] and experimental investigations [9], which have made wide range of applications in nanophotonics [5, 10-11].

An inverted cylindrical nanowire can be designed as a combination of two different semiconductor materials, having wider bandgap semiconductor as core, and smaller bandgap semiconductor as shell, as shown in fig 1. This novel imagination explores the possibility of tailoring microscopic attributes of the device by varying dimension configuration of different layers, as well as by varying the material constitution of core region also. This, in turn, effectively helps to provide the tuning of optoelectronic property of the device, thus making it as a potential candidate for future nano-photonic applications.

Since experimental quantum wires possesses finite potential barriers, energy eigenvalues may be near accurately computed only by applying suitable numerical methods for solution of the relevant envelope function equation. Thus appropriate numerical method plays a key role in determining the eigenstates of low-dimensional semiconductor structures. Various methods are already introduced by different workers in recent past for analyzing nanostructures having arbitrary potential profiles e.g., transfer-matrix technique [12], finite-element method [13], two-dimensional Fourier series [14], and finite-difference method [15]. Considering all these numerical techniques, finite difference method emerges out to be very efficient, as showed by Sullivan etc. [15-17].

Numerical computation for calculation of eigenstates of cylindrical core-shell nanowire was initiated by Wang [18] and Tkach [19] in recent past, and effect of field was also analyzed by workers [20]. Density of states function was computed [21] in presence of impurities. Carrier confinements in multi-shell 1D quantum devices were also computed [22] in analogy with core-shell structures. Effect of material parameters on photoluminescence spectra was analyzed by several researchers [23-24], and optical device was proposed for multishell [25] structures. Novel transistor device fabrication was already proposed [4, 6] which may bring a revolution in present VLSI technology.

In this paper, eigenstates and corresponding density of states of an inverted core-shell cylindrical quantum wire are computed using finite-difference method considering GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$  material composition, where  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  is considered as core material, and GaAs is dealt with as shell material. Three lowest eigenvalues are evaluated considering BenDaniel Duke boundary condition for effective mass mismatch at junctions, and conduction band discontinuity. Corresponding intersubband transition energies are calculated to study the lasing performance when it will be utilized as quantum wire laser. Calculation helps to analyze the absorption and emission spectra and their corresponding shift with variation of dimension and mole fraction.

## 2. Model

We consider schematic structure of a cylindrical nanowire as shown in fig 1. Schrödinger's equation for the quantum wire having circular cross-section can be written in Cartesian co-ordinate system as

$$-\frac{\hbar^2}{2m^*} \left[ \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] \psi(y, z) + V(y, z) \psi(y, z) = E_{y,z} \psi(y, z) \quad \dots(1)$$

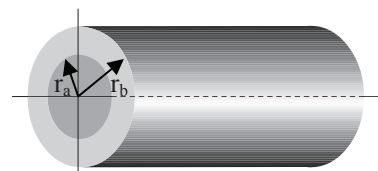


Figure 1. Schematic structure of core shell cylindrical quantum wire

Transforming into cylindrical coordinate system and due to independence of wavefunction on angular ordinate owing to circular symmetry, eq. (1) may be re-written as

$$-\frac{\hbar^2}{2m^*} \left[ \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} \right] \psi(r) + V(r)\psi(r) = E_r \psi(r) \quad \dots(2)$$

where  $E_r$  is the eigenvalue associated with the confined cross-sectional motion. After transformation in finite difference domain, eq. (3) may be modified as

$$\begin{aligned} \psi_r(j+1) \left[ -\frac{\hbar^2}{4m^* r(\delta r)} - \frac{\hbar^2}{2m^* (\delta r)^2} \right] + \psi_r(j) \left[ \frac{\hbar^2}{m^* (\delta r)^2} + V(r) \right] \\ + \psi_r(j-1) \left[ \frac{\hbar^2}{4m^* r(\delta r)} - \frac{\hbar^2}{2m^* (\delta r)^2} \right] = E_r \psi(r) \end{aligned} \quad \dots(3)$$

Solution of eq. (2) is used to determine eigenenergy for the core-shell structure, where core and shell regions are defined as

$$\begin{aligned} 0 < r_a \leq a \\ a < (r_b - r_a) \leq b \end{aligned} \quad \dots(4)$$

$a$  and  $b$  are radii of core and shell structures respectively. For analysis purpose, effective mass dependence on material parameter and conduction band discontinuity are also taken into account for near accurate result.

From dispersion relation, within the quantum wire with subband minima  $E_i$ , the density of states at any particular energy is the sum over all the subbands that can be written as

$$D(E) = \sum_{i=1}^n \frac{g_s g_v}{2\pi} \sqrt{\frac{2m^*}{\hbar^2}} (E - E_i)^{-0.5} \Theta(E - E_i) \quad \dots(5)$$

where  $g_s$  and  $g_v$  are spin and valley degeneracy respectively.

### 3. Results and discussion

Numerical computation is carried out on the inverted core-shell cylindrical quantum wire structure for estimation lower state eigenenergies and corresponding density of states. Also intersubband transition energies are calculated based on the eigenstates which provides a fair knowledge on the lasing performance of the device. For simulation purpose,  $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$  material composition is considered which adds the flexibility of modifying the material composition of core material from the perspective of design engineer's as it controls the photoemission characteristics alongside with the dimensional control of the structure.

Numerical analysis is initiated with the study of energy states with thickness of shell region for a constant outer radius of the structure. This is plotted in fig 2 where  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$  is considered as core material for 50 nm wire radius. It is observed that with smaller thickness, eigenvalue increases due to higher quantum confinement.

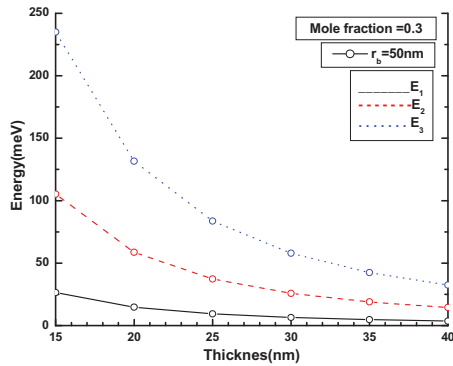


Fig. 2. Energy profile with thickness of shell region for  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$  structure with constant outer radius (50 nm)

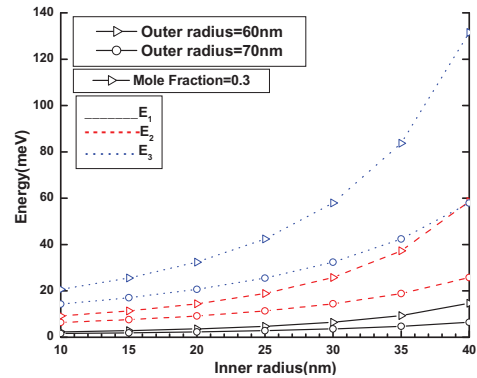


Fig. 3. Energy profile with radius of core region for  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$  structure with two different outer radii (60 nm & 70 nm)

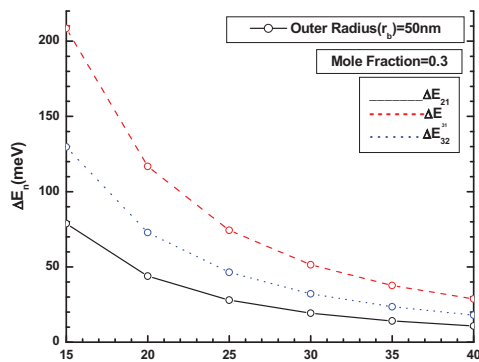


Fig. 4. Intersubband transition energy profile with thickness of shell region for  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$  structure with constant outer radius (50 nm)

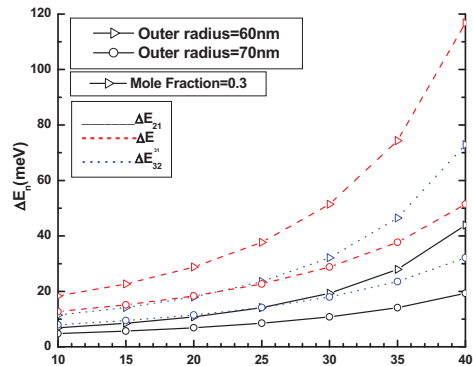


Fig. 5. Intersubband transition energy profile with radius of core region for  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$  structure with two different outer radii (60 nm & 70 nm)

If we consider the variation with core radius, then it shows the reverse trend for a specified material composition. This is shown in fig 3 for two different outer radii. It is obvious that with higher radius of the wire, eigenvalue becomes less, as depicted in figure. The change of eigenenergy with outer dimension is less significant for ground state, but is quite observable for higher states.

Corresponding intersubband transition energies are computed and their variations are plotted with respect to thickness of shell layer and core dimension independently. Fig 4 shows the intersubband energy profile with thickness. From the figure, it can be concluded that lower thickness provide higher transition energy, and thus lowers corresponding wavelength. Higher the difference between eigenstates, lower the emission wavelength, as expected. It increases with radius of core layer and becomes higher with lower dimension of the wire. This is also quite evident from knowledge of fig 3.

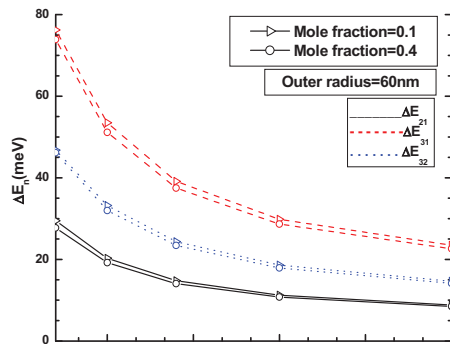


Fig. 6. Intersubband transition energy profile with ratio of outer-to-inner radii for constant outer radius with two different material compositions

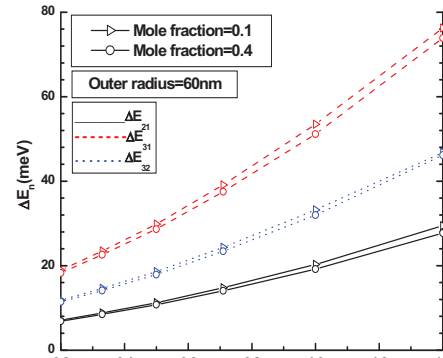


Fig. 7. Intersubband transition energy with ratio of core-radius-to-shell-thickness for constant outer radius with two different material compositions

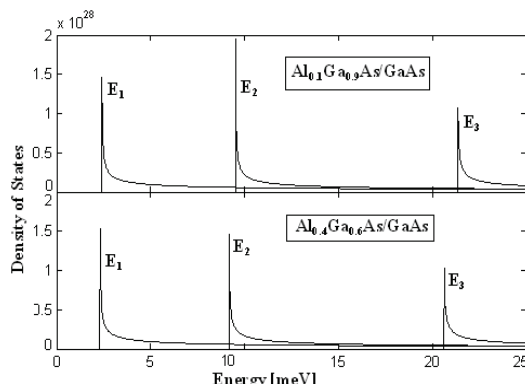


Fig.8. Density of states profile with energy for constant dimension with two different core materials

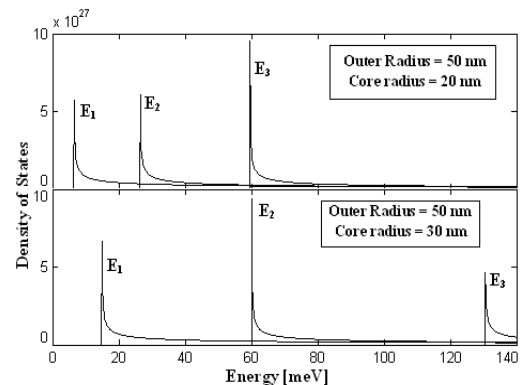


Fig.9. Density of states profile with energy for constant outer radius with two different core radii

Intersubband energies are also plotted with the ratio of outer to core radii for two different material compositions, as shown in fig 6 for a constant outer radius. This analysis emphasizes the importance of material parameter in optical tuning of the device as higher mole fraction reduces the transition energies. This is due to the fact that higher the Al composition in core layer, conduction bandgap discontinuity

Knowledge on density of states profile of the structure supports the observations. When it is evaluated with energy for two different mole fractions of Al, fig reveals the fact that shifts of eignestate is quite observable when higher states are considered than ground state. This is plotted in fig 8.

Fig 9 shows the DOS profile for varying core thickness. It can be concluded from the plot that higher dimension of core material gives higher energy, which effectively supports fig 3. It is evident from the figure that with higher dimension, confinement is better, as expected, and thus higher confinement leads to higher eigenenergies.

By increasing shell thickness and simultaneously keeping core radius constant, eigenvalue decreases due to lowering of quantum confinement. This is shown in fig 10 as also expected from fig 2.

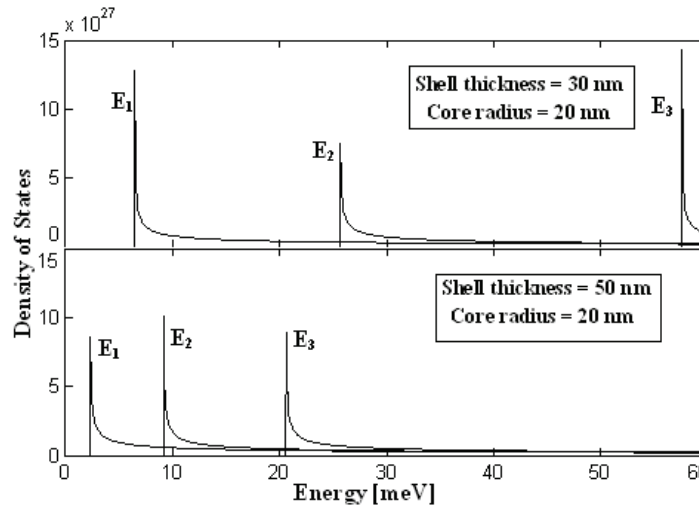


Fig 10: Density of states profile with energy for constant core radius with two different shell thicknesses

#### 4. Conclusion

The above analysis established the fact that dimensional control added with proper choice of material composition can suitably tailor the intersubband transition energies of an inverted core-shell cylindrical quantum wire. This presents a better alternative of novel quantum wire laser, possible with the development of fabrication technology. Dependence of eigenenergies for the lowest three states are studied on core radius, shell thickness and a variation of core material constitution within limit of type-I heterostructure. The above parameters modify the eigenstates which is also verify density of states profiles. Increasing the inner radius increases the eigenvalues with constant thickness, which signifies that wire's transition energies are enhanced as the wire itself is enlarged. This results a redshift in absorption and emission spectra, which can accurately be controlled at the time of manufacturing from the knowledge of material parameters and dimension. Increasing the shell thickness lowers carrier energies supported by DOS profile, which results a blueshift in optical transition spectra. Effect of simultaneous variation of both the core radius and shell thickness is also studied on intersubband transition energies. This is helpful for making a quantum wire laser using inverted core-shell structure from designer's perspective.

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